

Similar results have been found for other deformations. We find that some metallic-like nanotubes (labeled 5,5) remain conducting even when subjected to large compressive or tensile strain, as evidenced by their bandgaps remaining zero. However, other conducting tubes (labeled 9,0) develop sizeable band gaps under these conditions. Finally the band gaps of semiconducting tubes (8,0 and 10,0) are found to be very sensitive to the applied strain. Metallic nanotubes, such as the (5,5), retain their electronic properties even when subjected to large deformations; as a result, they are promising candidates for use in CNT-based electronic devices. On the other hand, other conducting tubes, such as the (9,0), are good candidates for MEMS devices, because their conductivity decreases markedly with increasing tensile strain. Optimal performance of CNT devices and sensors will be achieved by selecting the correct type of nanotube for the particular application.

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Computational Quantum Optoelectronics for Information Technology

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The interaction between laser light and semiconductor nanostructures is the basis for current and future optoelectronics-based information technology. The objective of the Computational Quantum Optoelectronics (CQP) project at Ames Research Center is to explore new optoelectronic devices, to study speed and size limits imposed by fundamental physics principles, and to design and optimize the performance of existing devices to meet NASA's needs in information technology. During FY99 the project made significant accomplishments in three areas: comprehensive semiconductor laser simulation, ultrafast laser modulation with a terahertz

heating field, and terahertz wave generation in semiconductor quantum wells.

In terms of comprehensive laser simulation, the focus in FY99 was on the so-called vertical-cavity surface-emitting laser (VCSEL). Ames researchers have developed a comprehensive simulation code using finite-difference methods in time and two-dimensional space domain. The model takes into account the quantum-well structure information and the material composition of a given VCSEL structure design. The effects of the detailed Coulomb interactions of charged carriers are also included. Since researchers directly solve the resulting partial differential equations numerically, VCSELs of different designs are treated with the same ease, such as those with gain confinement or index confinement, or devices of different current contact shapes. Also, time-evolution of VCSEL spatial modes on a picosecond scale are resolved. This type of space-time-resolved simulation is especially important when VCSELs are subject to injection current modulation, as is the case in VCSEL-based interconnects. Figure 1 shows the output laser intensity patterns at four different pumping levels for a VCSEL with an annular current contact.

In the area of ultrafast laser modulation, researchers have investigated the possibility of increasing the communication bandwidth by utilizing the much faster process of heating the electron-hole gas in a semiconductor with an electrical field. Detailed investigation has shown the feasibility and limitations of using such an approach. Researchers have investigated the underlying physical processes of electron-hole plasma interacting with semiconductor lattice vibrations when heated by an applied electrical field with frequency up to a few terahertz. They developed a detailed model to study laser modulation under such a terahertz-heating field. The results show that this method allows a modulation of semiconductor lasers at frequencies from tens of gigahertz (10^9 Hz) to 1 terahertz (10^{12} Hz). Even though it is a theoretical result at this stage, the approach indicates some fundamental advantages of this new modulation strategy over existing approaches.

Another closely related area of research in the overall effort in quantum optoelectronics is terahertz generation. We have investigated two possibilities using carefully designed quantum-well structures for

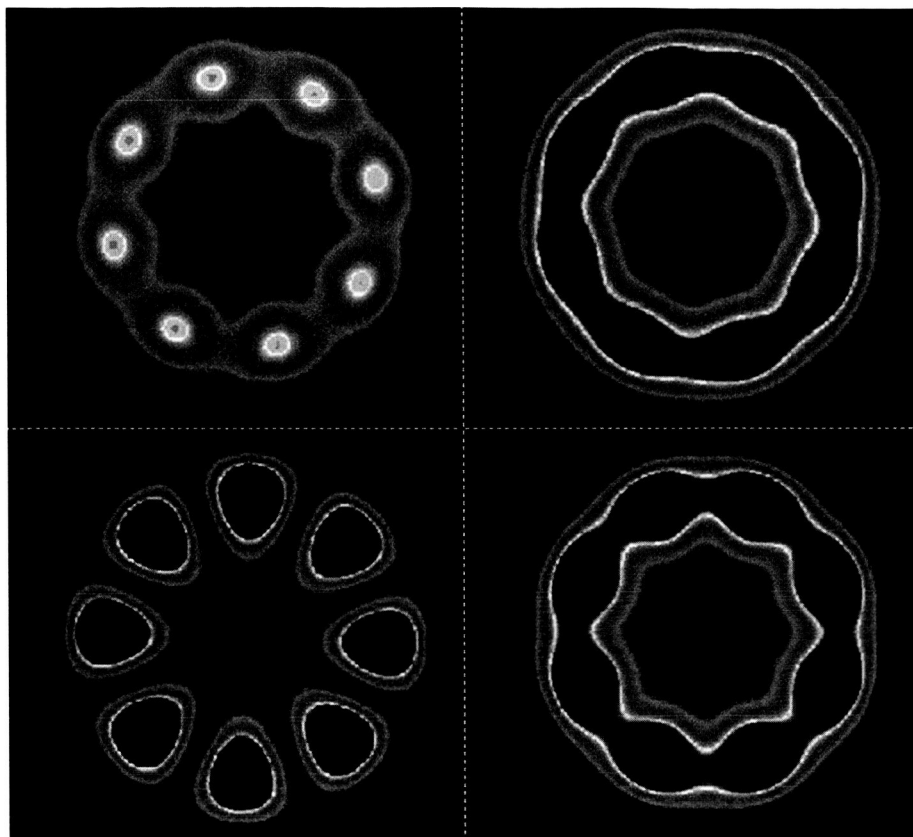


Fig. 1. The figure shows an example of the space-time-resolved computer simulation of the laser intensity pattern across the output facet. The four images show snapshots of the laser intensity at different times for a VCSEL with a current contact of the annular shape.

achieving terahertz emission through optical pumping by another laser. The first possibility is an optically pumped terahertz laser. The second approach is based on nonlinear optical wave mixing. Ames researchers have developed a theoretical model and computer simulation code that allows them to optimize the quantum-well structure design to achieve maximum nonlinear optical coefficients. Systematic theoretical and numerical simulation has shown the feasibility of generating radiation at a few terahertz by using this approach. This frequency is critical for the Earth Science Enterprise's atmosphere spectroscopy program and in far-infrared astronomy for the Space Science Enterprise. Efficient and compact terahertz sources will also find many commercial applications.

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A Liquifier for Mars Surface Applications

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NASA is planning an extensive set of robotic and human exploration missions that will make extensive use of cryogenic propellants. In-situ-consumable-production (ISCP) will reduce the mass launched from Earth by manufacturing propellant gases on the Mars surface. NASA's Exploration programs will benefit significantly from ISCP, providing that low cost, lightweight methods of propellant gas liquefaction are available to make exploration financially feasible.

The objective was to demonstrate that the planned 2003 Mars surface oxygen gas liquefaction requirement could be met with an existing, off-the-shelf tactical cryogenic cooler and a simple heat exchanger. The requirement is that oxygen gas produced during the daytime on the Mars surface